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THEORETICAL STUDIES OF DUST IN THE GALACTIC ENVIRONMENT: SOME RECENT ADVANCES

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ABSTRACT Dust grains, although a minor constituent, play a very important role in the thermodynamics and evolution of many astronomical objects, e.g., young and evolved stars, nebulae, interstellar clouds, and nuclei of some galaxies. Since the birth of infrared astronomy over two decades ago, significant progress has been made not only in the observations of galactic dust, but also in the theoretical studies of phenomena involving dust grains. Models with increasing degree of sophistication and physical realism (in terms of grain properties, dust formation, emission processes, and grain alignment mechanisms) have become available. Here I review recent progress made in the following areas:

1. Extinction and emission of fractal grains.
2. Dust formation in radiation-driven outflows of evolved stars.
3. Transient heating and emission of very small dust grains.

Where appropriate, relevant modeling results are presented and observational implications emphasized.

1. INTRODUCTION

In the early 1970's when infrared astronomy was in its infancy, many astrophysicists naturally became interested in the question of the composition, abundance, and origin of interstellar and circumstellar dust. George B. Field was among one of them and his papers (Field 1974, 1975) stimulated many discussions on the subject.

Since the birth of infrared astronomy over two decades ago, significant progress has been made not only in the observations of galactic dust, but also in the theoretical studies of phenomena involving dust grains. In the last decade, NASA has launched a number of space-based observatories: the Infrared Astronomical Satellite (IRAS), the Hubble Space Telescope, and the Cosmic Background Explorer. These space missions have stimulated advances in most branches of astrophysics and the data remain a vital resource for current research in infrared astronomy. To maximize the scientific returns of past and future space missions, complementary theoretical studies have also been undertaken. Models with increasing degree of physical realism have been constructed. The ultimate goal is to develop self-consistent physical models which can explain coherently present and future observations (Leung 1993).

Theoretical studies of phenomena involving galactic dust may be divided into several areas: (a) grain properties, (b) formation and destruction mechanisms, (c) emission processes and energetics, (d) grain alignment mechanisms, (e) grain surface chemistry. To demonstrate the progress made in some of these studies, I describe a few selected results in the following topics: (1) extinction and emission of fractal grains, (2) dust formation in radiation-driven outflows of evolved stars, and (3) transient heating and emission of very small dust grains.

2. SOME RECENT ADVANCES

2.1 Fractal Dust Grains

In astrophysical environments dust grains have irregular shapes most likely formed by fractal growth processes, i.e., stochastic growth processes leading to grains of irregular shapes. On the other hand, spherical dust grains are often assumed in models of infrared sources so that the dust opacity can be calculated from the Mie scattering theory. A computational technique now exists for calculating the dust opacity for grains of irregular shapes (Purcell & Pennypacker 1973; Draine 1988). In this method, called "discrete dipole approximation" (DDA), an irregularly shaped grain is approximated by a collection of dipoles. The DDA is valid only when the dipole lattice spacing (Δ) is less than the wavelength of the incident radiation. For a fractal grain approximated by N dipoles, $\Delta = (4\pi/3N)^{1/3}\, a_{eff}$, where a_{eff} is the radius of a sphere containing the same number of dipoles. For $a_{eff} = 0.1$ μm and $N = 512$, the DDA introduces typical errors of 5% in spectral regions where the approximation is valid.

Before calculating the grain opacity using the DDA, one must determine the grain shape by computer simulation. Two limiting examples of fractal growth processes are particle-particle aggregation and cluster-cluster aggregation (Witten and Cates 1986). In particle-particle aggregation, also known as diffusion limited aggregation (DLA), grain growth proceeds randomly by adding one basic unit (monomer) at a time. In cluster-cluster aggregation (CCA), grain growth starts with an ensemble of N monomers which proceed to form at random an ensemble of N/2 dimers, which in turn form an ensemble of N/4 tetramers and so on. This process continues until a single grain is formed after $M = \log_2(N)$ steps. In terms of morphology, a DLA grain is more compact than a CCA grain which has more open and filamentary structure.

While the general effects of grain topology and compositional inhomogeneities on the extinction cross sections of fractal grains have been studied (Wright 1987; Bazell and Dwek 1990), attempts to characterize the thermal, radiative, and observable properties of irregularly shaped grains have not been made until recently (Fogal & Leung 1994). A useful parameter to characterize the topology of irregularly shaped grains is fractal dimension (D), defined by the relation $N(r) \sim r^D$, where N(r) is the number of monomers within a sphere of radius r. For a spherical grain, D = 3. For a rod shaped grain, D = 1. In general $1 < D < 3$ and the smaller the fractal dimension, the more filamentary the structure. For DLA grains, D = 2.5 while for CCA grains, D = 1.8 - 2.2. Recent studies (Fogal & Leung 1994) show that the thermal and radiative properties of a dust grain depends on the ratio (p) of volume to surface area, which is determined by the fractal dimension D (see Figure 1). For a given mass, grains with the same D, independent of detailed shape, show almost no difference in their absorption cross sections, temperature, and energy spectrum. *Hence in modeling phenomena involving irregularly shaped grains, we need to introduce just one parameter, the fractal dimension D, to characterize the shape.* It should be emphasized that porosity [P = 1 - (volume of solid)/(total volume)] and fractal dimension need not be uniquely related. Porosity measures the effect of volume filling factor in a grain and is ill-defined for a dust grain with open and filamentary structure. Grains with the same porosity may have very different fractal dimensions and vice versa.

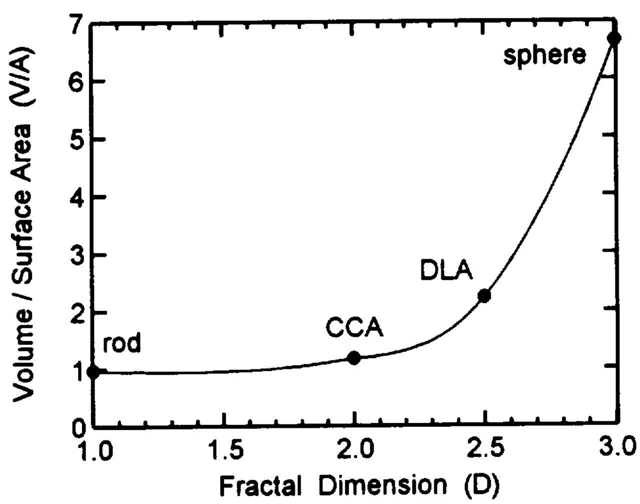

FIGURE 1 Fractal dimension vs. volume to surface area (normalized by some constant) for dust grains of different shapes: rod, cluster aggregate (CCA), particle aggregate (DLA), and sphere.

The exact details of grain nucleation and growth determine the fractal dimension, which in turn may affect the intensity and shape of spectral features in the energy spectrum of infrared sources. For example, the intensity ratio of the 10 and 20 μm silicate features in the flux spectrum decreases with D, i.e., compared to spherical grains, fractal grains are less compact and being cooler, will emit more strongly at long wavelengths, leading to a lower ratio of the 10 and 20 μm silicate features. Hence observed spectral profiles may be an important diagnostic for deducing the fractal dimension of dust grains formed in stellar outflows. This in turn will shed light on our understanding of dust formation.

There are several important astrophysical consequences of removing the unrealistic assumption of spherical grains:

(1) Fractal grains are cooler than spherical grains (typically by 10-20%) so that radiation transport models of infrared sources with fractal grains would show a shift in the peak flux toward longer wavelengths (Fogal & Leung 1991). Since cooling by emission increases with grain surface area, fractal grains, being less compact and have a lower ratio of volume to surface area, attain lower temperatures. Consequently determination of dust column density based on models assuming spherical grains would lead to overestimate.

(2) Since fractal grains generally have larger extinction cross sections (compared to spherical grains of the same composition and volume), models of the interstellar extinction curve using fractal grains (instead of spherical grains) require less elemental depletion, typically by one-third (Fogal & Leung 1993). Specifically the model of interstellar extinction by Mathis, Rumpl, and Nordseick (1977) as applied by Draine and Lee (1984) requires 58%, 90%, 95%, 94%, and 16% respectively of the total cosmic abundance of C, Si, Mg, Fe, and O. On the other hand, a model using fractal grains (CCA grains) requires only 45%, 66%, 68%, 64%, and 11% respectively of these elements. This is due to the fact that less mass is required for fractal grains to produce the same extinction as spherical grains.

(3) In the studies of radiation-driven mass loss in evolved stars, both the mass loss rates and details of outflow dynamics need to be revised since radiation pressure on dust depends sensitively on the extinction cross sections of newly formed grains.

2.2 Dust Formation in Stellar Outflows

A key theoretical problem related to circumstellar dust envelopes around evolved stars is the formation of dust grains and its impact on the mass loss phenomenon. Since dust grains would condense out of the gas as it cools down on its way out of the star, the dominant mechanism for mass loss should be radiation pressure which can drive the dust and surrounding gas outward through momentum coupling. In the warm circumstellar environment, very small grains are unstable to evaporation or sublimation (i.e., more likely to become smaller by losing one or more atoms than to grow by accreting one or more atoms): there is therefore a barrier to grain formation which must be overcome by nucleation. Grain formation in outflows thus consists of nucleation followed by growth. While the kinetic equations governing nucleation (master equations) are well known, the large number of monomers per grain has made this type of study of nucleation impractical. As an alternative, most studies have used the classical nucleation theory (cf., Draine and Salpeter 1977, Yamamoto and Hasagawa 1977) to describe the formation of the initial molecular clusters out of a slowly cooling vapor, generally under the assumption of LTE. The growth rate of such clusters is then estimated from their free energies. The growth of condensation nuclei can then be determined by the solution of a system of differential equations involving moments of the grain size distribution (Gail and Sedlmayr 1988). This method efficiently calculates the average properties of dust grains in stellar outflows. The moment equations, however, are highly dependent on the nucleation rate of particles in the gas. Since the circumstellar environment is far from thermodynamic equilibrium, and because relatively complex chemistry may be involved (e.g., in the formation of small "silicate" clusters), the use of classical nucleation theory is highly suspect.

A promising approach (Vicanek & Ghoniem 1992) is to solve a truncated set of kinetic equations (which govern small cluster growth or nucleation) simultaneously with the moment equations (which determine the growth of large particles), thus allowing a self-consistent treatment of grain nucleation and growth. The grain size distribution function is then reconstructed from its moments using a method based on the maximum entropy principle. To test the validity of classical nucleation theory in astrophysical environments, this approach has been applied (Egan & Leung 1993) to study the problem of homogeneous dust formation in carbon stars. It is found that classical nucleation theory is not well suited to circumstellar environments. Independent of mass-loss rates, it predicts nucleation of grains to occur at a much lower supersaturation than is calculated from the kinetic equations, thus predicting dust formation too close to a star, overestimating the number of dust grains produced, and underestimating the average grain size. Results also indicate that coagulation of clusters is not important for high mass-loss situations because the high density of monomers leads to very rapid grain growth once nuclei form. In models with lower mass-loss rates, the addition of larger clusters becomes important in grain growth. Including these processes lowers the supersaturation ratio at which grains formed since coagulation facilitates the formation of grain nuclei. Furthermore, including particle drift velocities increases the collisional rates, thus allowing grain formation to occur at a lower supersaturation ratio. Finally, it is found that the number, size and supersaturation ratio at which grains form depends sensitively on the outflow velocity (Figure 2). For small outflow velocities (1 km/s), grains form close to the stellar photosphere and at a low supersaturation ratio. Large grains are formed but with smaller number densities. At higher velocities (> 10 km/s), grains form farther from the stellar photosphere and at a higher supersaturation ratio. Although the grains formed are much smaller, a larger numbers of them are produced.

To study the effects of grain formation on the dynamics of stellar outflows and vice versa, one must incorporate self-consistently the momentum transfer between gas and dust. This requires the simultaneous solution of the fluid dynamics equations and the equations of grain nucleation and growth (Egan, Leung & Coffin 1993). These time-dependent models indicate that grain formation is a two-stage process, with large grains forming close to the stellar photosphere and evaporating to much smaller sizes as they are accelerated by radiation pressure into lower density regions (Egan 1994). As the expanding gas cools, formation of additional small grains occurs. The velocity structure of the circumstellar shell consists of a number of shocks corresponding to bursts of grain formation. The effects of different [C]/[O] ratios, stellar temperature and stellar luminosity are also investigated. Results from time-dependent models indicate that a higher [C]/[O] ratio lead to higher mass-loss rates. Furthermore, contrary to common perception, higher stellar luminosities actually lead to *lower* mass-loss rates because only small grains are formed.

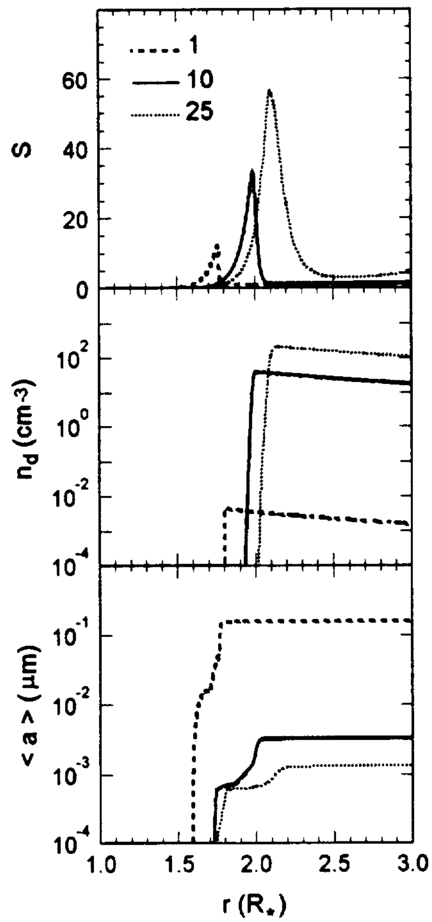

FIGURE 2 Effect of outflow velocity on the radial dependence of the supersaturation ratio (S), number density (n_d), and average grain size (< a >). The outflow velocities are respectively 1, 10, 25 km s^{-1}.

2.3 Emission Processes

Among the unexpected results from IRAS was the discovery of excess mid-infrared (MIR) emission detected in many infrared sources, e.g., diffuse clouds, dark globules, visual reflection nebulae, and high-latitude dust clouds or infrared cirrus (for a review see Puget and Leger 1989). This excess MIR emission is always accompanied by relatively high color temperatures derived from the 12 to 25 μm flux ratio. They are typically ten times higher than those from the 60 to 100 μm flux ratio. It is now believed that the emission at short wavelengths (< 30 μm) comes from transient heating of very small grains, large polycyclic aromatic hydrocarbons (PAHs), or hydrogenated amorphous carbons (HACs).

The physics of interstellar grain heating and temperature (Figure 3) is governed by a heating parameter (x), defined as the ratio of the heat capacity of grain to the energy of photon absorbed. For classical large grains (grain size $a \geq 0.1$ μm), $x >> 1$ while $x << 1$ for very small grains ($a < 50$ Å). Thermal emission from classical grains exposed to the interstellar radiation field (ISRF) is modeled assuming the grain temperature is time independent, being established by the local energy balance between heating due to photoabsorption and cooling due to thermal emission. Under this assumption, which is equivalent to the assumptions of LTE and radiative equilibrium in modeling stellar atmospheres, a single grain temperature is valid locally for an ensemble of identical grains. This assumption breaks down, however, when the energy of the heating photons becomes comparable to the total energy content of a dust grain. In this case ($x < 1$), the grain temperature will fluctuate with time: the grain heats up rapidly following a discrete heating event and gradually cools down until the next interaction occurs. For transient heating a dust grain can attain temperatures much higher than those predicted by the equilibrium assumption. Furthermore, instead of a single temperature, a distribution of temperatures, described by a probability density function, exist at a given time for an ensemble of identical grains. Temperature fluctuations in small grains can change significantly the energy distribution of the radiation field in infrared sources.

To calculate the temperature probability distribution in transient heating, we divide the allowed enthalpy range into a number of discrete bins. A rate matrix is set up with transition rates involving discrete heating and continuous cooling processes between different bins. This leads to a system of linear equations similar to the equations of statistical equilibrium for determining level populations of the energy levels in a molecule (Guhathakurta & Draine 1989). Typically 150 to 250 bins or energy levels are required. Using this approach we can solve the radiation transport problem involving transient heating as a non-LTE line transfer problem involving many transitions (Lis & Leung 1991a, Siebenmorgen, Krugel & Mathis 1992). Compared to equilibrium heating which can be solved as a LTE continuum transfer problem, modeling transient heating increases the computing requirement typically by a thousandfold.

Using this approach detailed models can now be constructed which treat self-consistently the thermal coupling between the transient heating of small grains and the equilibrium heating of classical large grains. Such radiation transport models have been used to interpret the IRAS observations of the Barnard 5 cloud (Lis & Leung 1991b) and a diffuse cloud in Chamaeleon (Doty, Leung & Lis 1994a). In both cases, longward of 100 μm, the emission is dominated by large grains. Between 30-100 μm, the emission is produced mainly by very small grains. Shortward of 30 μm, both

PAHs/HACs and small grains are responsible for the emission. Typically very small grains and PAHs/HACs account for 10-20% of the total opacity in the visible, and 5-20% of the total dust mass of the cloud. Furthermore, to produce the observed infrared limb brightening, the spatial distribution of small grains and PAHs must be more extended than that of large grains. The existence of a halo of very small grains and PAHs/HACs around interstellar clouds has important significance in understanding the origin of small grains and PAHs/HACs.

MODELING INTERSTELLAR GRAIN HEATING & TEMPERATURES

	Classical Large Grains	Very Small Grains
typical size	• ~ 0.1 μm	• < 50 Å
heating parameter	• large (x >>1)	• small (x <<1)
heating	• continuous (equilibrium)	• transient (non-equilibrium)
temperature	• constant (delta function)	• fluctuating (distribut. function)
temp. from ISRF	• about 20 K	• 10 - 100 K
spectrum peak	• > 100 μm	• 10 - 100 μm
radiation transport	• LTE continuum transfer	• NLTE line transfer
computing time	• about 6 Mflop-minutes	• about 6000 Mflop-minutes
computing hardware	• scalar machines	• vector/parallel machines

FIGURE 3 Schematic diagram comparing the modeling of grain heating and temperatures of interstellar grains: classical large grains vs. very small grains.

The need to incorporate transient heating of very small grains in radiation transport models can lead to ambiguities in the interpretation of infrared observations of interstellar clouds, e.g., in the study of dark globules which are nearby dense interstellar clouds primarily heated externally by the ISRF. Many dark globules show an excess in the MIR which has generally been attributed to an internal heat source (e.g., a protostellar object), since conventional large grains heated by the ISRF cannot account for the MIR excess. However, very small grains, if present, may be responsible for the MIR excess through transient heating by the ISRF. In such a case, the postulation of an internal heat source is not necessary. To quantitatively determine whether a MIR excess in dark globules uniquely implies the presence of an internal heat source, Doty, Leung & Lis (1994b) have modeled B335, a source known to have a 60 μm excess and an internal heat source. The observational data are compared with the results of two models: an internally heated one with only classical large grains, and an externally heated one with both large and very small grains. Both models can reproduce the observed flux spectrum (Figure 4), implying that a MIR excess in the flux spectrum of dark globules does not uniquely imply the presence of an internal heat source. The parameters for both models are within observational constraints. However, for sources which can be resolved, the surface brightness at 60 μm may be used as a diagnostic to differentiate between these two cases. Internally heated sources show extra emission at the center, and strong short wavelength emission at smaller radii. Externally heated sources, on the other hand, show less emission at the center of the cloud, and limb brightening at shorter wavelengths.

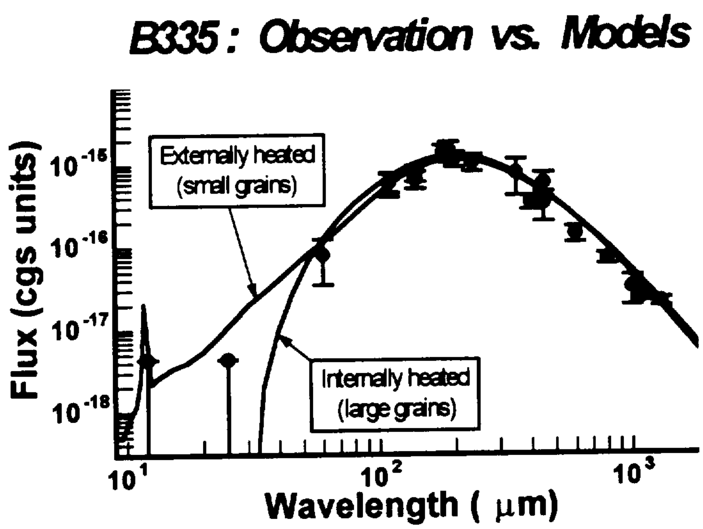

FIGURE 4 Comparison between observations of the dark globule B335 and results from two models: one with only classical large grains heated internally by an embedded energy source, and one with both large and very small grains heated externally by the ISRF. Both models can reproduce the observations reasonably well.

3. CONCLUSION

To summarize, in the last decade much progress has been made in the theoretical studies of dust in the galactic environment. Models with increasing degree of physical realism have become available. Future research should include other important physical processes so that self-consistent physical models can ultimately be constructed: a) transfer of polarized radiation, b) radiation hydrodynamics, c) radiation transport in 3-D geometry, d) heterogeneous grain nucleation and growth, and e) gas-phase and grain-surface chemistry. In addition, improvements in computational techniques, e.g., better algorithms and iteration procedure, should be made.

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REFERENCES

Bazell D., & Dwek, E. 1990, *ApJ*, **360**, 142

Doty, S. D., Leung, C. M., & Lis, D. C. 1994a, in *The First Symposium on the Infrared Cirrus and Diffuse Interstellar Clouds*, eds. R. M. Cutri & W. B. Latter, ASP Conference Series Vol. 58, p. 408

____________. 1994b, *BAAS*, **26**, 883

Draine, B. T. 1988, *ApJ*, **333**, 848

Draine, B. T., & Lee, H. M. 1984, *ApJ*, **285**, 89

Draine, B. T., & Salpeter, E. E. 1977, *J. Chem. Phys.*, **67**, 2230

Egan, M. P. 1994, *BAAS*, **26**, 925

Egan, M. P., & Leung, C. M. 1993, in *Astronomical Infrared Spectroscopy: Future Observational Directions*, ed. S. Kwok, ASP Conference Series Vol. 41, p. 221

Egan, M. P., Leung, C. M., & Coffin, D. J. 1993, *BAAS*, **25**, 1313

Field, G. B. 1974, *ApJ*, **187**, 453

____________. 1975, in *The Dusty Universe*, ed. G. B. Field & A. G. W. Cameron, Neale Watson Academic Publications, Inc., p, 89

Fogel, M. E., & Leung, C. M. 1991, *BAAS*, **23**, 1368

____________. 1993, *BAAS*, **25**, 1434

____________. 1994, in preparation

Gail, H. P., & Sedlmayr, E. 1988, *A&A*, **206**, 153

Guhathakurta, P., & Draine, B. T. 1989, *ApJ*, **345**, 230

Leung, C. M. 1993, in *Astronomical Infrared Spectroscopy: Future Observational Directions*, ed. S. Kwok, ASP Conference Series Vol. 41, p. 189

Lis, D. C., & Leung, C. M. 1991a, *Icarus*, **91**, 7

____________. 1991b, *ApJ*, **372**, L107

Mathis, J. S., Rumpl, W., & Nordsieck, K. N. 1977, *ApJ*, **217**, 425

Purcell, E. M., & Pennypacker, C. R. 1973, *ApJ*, **186**, 705

Puget, J. L.,& Leger, A. 1989, *ARA&A*, **27**, 161

Siebenmorgen, R., Krugel, E., & Mathis, J. S. 1992, *A&A*, **266**, 501

Vicanek, M., & Ghoniem, N. M. 1992, *J. Comp. Phys.*, **101**, 1

Witten, T. A., & Cates, M. E. 1986, *Science*, **232**, 1607

Wright, E. L. 1987, *ApJ*, **320**, 818

Yamamoto, T., & Hasegawa, H. 1977, *Prog. Theor. Phys.* **58**, 816